LISTING OF CLAIMS

This listing of claims will replace all prior versions, and listings, of claims in this application.

1. (currently amended) A method of using parallel computational means to determine the three-dimensional structure of a molecule of interest from experimental X-ray diffraction data for a crystal of said molecule of interest, which comprises

(a) selecting as a basis set an orthogonal set of at least one spherical harmonic spherical Bessel basis function to represent the three dimensional electron density in said crystal, thereby generating a spherical harmonic spherical Bessel model, such that the number of degrees of freedom in the electron density of the model is reduced relative to the number of experimental data;

(b) determining the maximum minimal resolution of said spherical harmonic spherical Bessel model to be used to determine the three-dimensional structure of said molecule of interest;

(c) determining a radius and position for a spherical asymmetric unit in a model crystal lattice as derived from said experimental X-ray diffraction data for said crystal;

(d) determining a computationally efficient grouping of x-ray diffraction intensities for the positioning of at least one spherical harmonic spherical Bessel basis function;

(e) modifying at least one spherical harmonic spherical Bessel basis function within the basis set selected in (a) such that it represents an individual basis

function centered at a specific position and ~~becomes~~ can be converted into a Fourier representation of a positionally translated basis function;

(f) calculating said at least one Fourier representation of a full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function for each basis function in the basis set selected in (a);

(g) determining by parallel computational means at least one ~~complex-valued~~ coefficient, which comprises a complex number, of said spherical harmonic spherical Bessel basis function by comparing said full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function calculated in (f) with said experimental x-ray diffraction data, wherein scale factors and correlation coefficients of the phase angle of said complex-~~valued~~number coefficient are calculated at ~~any one of the set of presumed values~~ phase angle values of 0° ~~and~~ or 90°;

(h) using said at least one ~~complex-valued~~ coefficient, which comprises a complex number, of each spherical harmonic spherical Bessel basis function in the basis set selected in (a) for said spherical harmonic spherical Bessel basis function to iteratively update a phased Fourier representation of the three-dimensional electron density of said crystal;

(i) calculating Fourier summations based on a combination of said phased Fourier representation and the x-ray diffraction intensities to obtain an interpretable three-dimensional representation of the contents of the full-unit cell; and

(j) outputting said three-dimensional representation to a suitable output hardware.

2. (currently amended) The method of claim 1, further comprising, subsequent to step (i), the additional steps of:

(j) determining a three-dimensional model structure of said molecule of interest by computational graphical model fitting; and

(k) subjecting said three-dimensional model structure to ~~improvements by~~ simulated annealing, least squares, maximum entropy, and/or Bayesian data analysis and/or molecular mechanics energy minimizations.

3. (previously presented) The method of claim 1, wherein said radius and position for said spherical asymmetric unit is known.

4. (previously presented) The method of claim 1, wherein said radius and position for said spherical asymmetric unit is not known.

5. (previously presented) The method of claim 4, further comprising, prior to step (j), the step of determining radius and position of the largest spherical asymmetric unit that can fit into a predetermined crystal lattice without overlap.

6. (previously presented) The method of claim 5, further comprising, prior to step (j), the step of determining the numerical value of the angular increment between each trial value estimated for the phase angle of coefficient of a spherical harmonic spherical Bessel component basis function of a model generated from said largest spherical asymmetric unit.

7. (currently amended) The method of claim 5, further comprising, prior to step (j), the step of determining the value of the complex-~~valued~~number coefficient of said spherical harmonic spherical Bessel basis function.

8. (previously presented) The method of claim 1, further comprising, prior to step (j), the step of determining the total number of m-indices to be provided to a recursive calculation.

9. (currently amended) The method of claim 1, further comprising, prior to step (j), the step of determining a starting and a final value of an arbitrary exponent by which power to raise the values of said calculated correlation coefficients ~~to allow iterative improvement of the electron density of the model~~.

10. (previously presented) The method of claim 1, further comprising, prior to step (j), the step of determining said at least one spherical Bessel function together with ordinate values of a Bessel function argument such that the zeroes of these Bessel functions are calculated.

11. (previously presented) The method of claim 8, further comprising, prior to step (j), the step of converting said m-indices to spherical coordinates and initializing said numerical values associated with said m-indices to allow later recursive calculation of a value of

each spherical harmonic spherical Bessel basis function at said m-indices.

12. (previously presented) The method of claim 11, further comprising, prior to step (j), the step of executing a recursive program cycle wherein unphased diffraction amplitudes are converted to a Fourier transform of a calculated model of a portion of said full-unit cell.

Claim 13. (canceled).

14. (previously presented) The method of claim 1, wherein said method for determining the three-dimensional structure of said molecule of interest is carried out by a computer, said computer being capable of receiving data and performing said method.

15. (previously presented) The method of claim 14, wherein said computer is coupled to a display device and there exists a means for presenting the chemical or molecular structural characteristics of said at least one molecule of interest on said display device.

16. (original) The method of claim 1, wherein said at least one molecule of interest is selected from the group consisting of:

a) a pharmaceutical;
b) an enzyme;
c) a catalyst;
d) a polypeptide;
e) an oligopeptide;
f) a carbohydrate;

g) a nucleotide;

h) a macromolecular compound;

i) an organic moiety of an alkyl, cycloalkyl, aryl, aralkyl or alkaryl group or a substituted or heterocyclic derivative thereof;

j) an industrial compound;

k) a polymer;

l) a monomer;

m) an oligomer;

n) a polynucleotide;

o) a multimolecular aggregate; and

p) an oligopeptide.

17. (previously presented) The method of claim 1, wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the features of said molecule of interest such that said representation could be used to determine desirable chemical characteristics of said molecule of interest.

18. (previously presented) The method of claim 1, wherein the structural characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the features of said molecule of interest such that said representation could be used to determine structural characteristics of said molecule of interest that could be modified.

19. (original) The method of claim 1, wherein said method is further utilized to predict the chemical activity of at least one molecule of interest.

20. (original) The method of claim 1, wherein said method is further utilized to predict the biochemical activity of at least one molecule of interest.

21. (original) The method of claim 1, wherein said method is further utilized to predict the physiological activity of at least one molecule of interest.

22. (previously presented) The method of claim 1, further comprising depicting a three-dimensional structure of said molecule of interest from the summation of said at least one Fourier representation.

23. (previously presented) The method of claim 22, further comprising generating a three-dimensional model structure of said molecule of interest from said three-dimensional structure of said molecule of interest from the summation of said at least one Fourier representation.

Claims 24-36 (canceled).

37. (previously presented) The method of claim 1, wherein said x-ray diffraction data for said crystal further comprises data representing the crystal space group, the crystal symmetry operators, the crystal lattice dimensions and angles, the maximum resolution of the experimental diffraction data, the experimentally measured

values of the x-ray diffraction intensities, the derived values of the x-ray structure factor amplitudes, and an input value chosen from the maximum minimal resolution of the spherical harmonic spherical Bessel model of said molecule of interest.

Claim 38 (canceled).

39. (currently amended) The method of claim 1, further comprising, prior to step (j), the step of inputting a numerical value for the angular increment between each trial value presumed for the phase angle the ~~complex valued~~ coefficient, which comprises a complex number, of said spherical harmonic spherical Bessel basis function.

40. (currently amended) The method of claim 39, further comprising, prior to step (j), the step of determining an appropriate value of said angular increment automatically for each phase angle of the ~~complex valued~~ coefficient, which comprises a complex number, of said spherical harmonic spherical Bessel basis function.

41. (previously presented) The method of claim 1, further comprising, subsequent to step (i), the additional steps of:

(j) determining, from the input limiting resolution for the spherical harmonic spherical Bessel model, the extent of the indices *lmn* of the spherical harmonic spherical Bessel basis function that are required for said molecule of interest;

(k) converting diffraction indices (hkl) to spherical coordinates;

(l) initializing some numerical values associated with each diffraction index to allow later recursive calculation of the value of each spherical harmonic spherical Bessel basis function at each hkl index; and

(m) executing a recursive program cycle.

42. (previously presented) The method of claim 41, further comprising, subsequent to step (m), the additional steps of:

(n) inputting the observed experimental diffraction amplitudes for each hkl index in the Fourier representation;

(o) converting a set of spherical harmonic spherical Bessel coefficients to at least one Fourier representation; and

(p) combining the contributions from the l, m, and n components of said at least one Fourier representation of the spherical harmonic spherical Bessel basis function to provide a full three-dimensional Fourier representation of the spherical harmonic spherical Bessel basis function of said molecule of interest.

43. (original) The method of claim 1, further comprising, prior to step (j), the step of writing information concerning the three dimensional Fourier representation of the model of said crystal of said molecule of interest to an electronic record keeper, thereby storing the spherical harmonic spherical Bessel model, including the Fourier representation of each stored spherical harmonic spherical Bessel model such that it may

be read at the beginning of the calculation for the next packet of m-values for the m-indices.

44. (previously presented) The method of claim 1, wherein the steps and calculations necessary for rendering the three-dimensional representation of said molecule of interest are capable of being recorded in an electronic medium.

45. (previously presented) The method of claim 1, wherein the steps and calculations necessary for the rendering the three-dimensional representation of said molecule of interest are recorded in an electronic medium and stored in a secondary storage device.

46. (previously presented) The method of claim 1, wherein said suitable output hardware is a monitor.

47. (previously presented) The method of claim 43, wherein said method further provides a computational means to record the steps of the method, wherein said means is selected from the group consisting of:

a) a floppy disk;
b) a second hard disk drive;
c) a read/write compact disc;
d) magnetic tape;
e) a Bernoulli Box;
f) a Zip disk; and
g) other means for storing electronic data.

48. (currently amended) A method of using parallel computational means to determine the three-

dimensional structure of a molecule of interest from experimental X-ray diffraction data for a crystal of said molecule of interest, comprising the steps of:

(a) choosing, as the basis set, an orthogonal set of at least one spherical harmonic spherical Bessel basis function to represent the three-dimensional electron density in the crystal, thereby generating a spherical harmonic spherical Bessel model, such that the number of degrees of freedom in the electron density of the model is reduced relative to the number of experimental data;

(b) determining the maximum minimal resolution of said spherical harmonic spherical Bessel model to be used to determine the three-dimensional structure of said molecule of interest;

(c) determining a radius and position for a spherical asymmetric unit in a model crystal lattice as derived from said diffraction data for said crystal;

(d) determining a computationally efficient grouping of x-ray diffraction intensities for the positioning of at least one spherical harmonic spherical Bessel basis function;

(e) modifying at least one spherical harmonic spherical Bessel basis function within the selected basis set such that it represents an individual basis function centered at a specific position and ~~becomes~~ can be converted into a Fourier representation of a positionally translated basis function;

(f) calculating said at least one Fourier representation of a full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function for each basis function in the basis set chosen in (a);

(g) determining by parallel computational means at least one ~~complex valued~~ coefficient, which comprises a complex number, of said spherical harmonic spherical Bessel basis function by comparing said full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function determined in (f) with said experimental x-ray diffraction data, wherein scale factors and correlation coefficients of the phase angle of said complex-~~valued~~number coefficient are calculated at ~~any one of the set of presumed values~~ phase angle values of 0° ~~and~~ or 90°;

(h) using said determined coefficients of each spherical harmonic spherical Bessel function in the basis set for said spherical harmonic spherical Bessel function to update iteratively a phased Fourier representation of the three-dimensional electron density of the crystal;

(i) calculating Fourier summations based on a combination of said phased Fourier representation and the x-ray diffraction intensities to obtain an interpretable three-dimensional representation of the contents of said full-unit cell; and

(j) outputting said three-dimensional representation to a suitable output hardware;

wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the molecular features of said molecule of interest such that said representation could be used to alter the chemical characteristics of said molecule of interest.

49. (canceled) The method of claim 48 wherein said spherical harmonic model to be used is the spherical Bessel mode.

50. (previously presented) The method of claim 48, wherein said radius and position for said spherical asymmetric unit is known.

51. (previously presented) The method of claim 48, wherein said radius and position for said spherical asymmetric unit is not known.

52. (original) The method of claim 48, further comprising the step of writing information concerning the three dimensional structure of said molecule of interest to an electronic record keeper, the Fourier representation of each stored spherical harmonic spherical Bessel model such that it may be read at the beginning of the calculation for the next packet of m-values for the m-indices.

53. (previously presented) The method of claim 48, wherein the steps and calculations necessary for determination of the representation of said molecule of interest is capable of being recorded in an electronic medium.

Claims 54-60 (canceled).

61. (previously presented) The method of claim 48, wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation

allowing the identification of the molecular features of said molecule of interest such that said representation could be used to alter to the chemical characteristics of said molecule of interest.

62. (original) The method of claim 48, wherein said method is further utilized to predict the chemical activity of at least one molecule of interest.

Claims 63-69 (canceled).